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Computation of the dipole moment of some heteronuclear diatomic molecules in terms of the revised electronegativity scale of Allred and Rochow

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ABSTRACT

Recently we have calculated the electronegativity of 103 elements of the periodic table relying upon the basic approach of Allred and Rochow. We carefully allayed the dimensional mismatch seemingly prevalent in all previous calculations so that the computed electronegativity is in its proper force dimension. Since the electronegativity is neither a physical observable nor a quantum mechanically determinable quantity, there is no benchmark to perform any validity test of any scale of electronegativity. The descriptors of the real world such as charge distribution, bond energies, bond polarities and the dipole moments, force constants, atomic polar tensor and internuclear distances can be conceived in terms of electronegativity. Since the scale of Allred and Rochow is extremely popular among the scales of electronegativity, we have performed a validity test of the newly modified scale by calculating the dipole moments of as many as 48 molecules of widely diverse nature using the electronegativity values computed by us. The comparative study of computed dipole moments vis-à-vis the available experimental dipole moments of the corresponding molecules reveals that the present scale of electronegativity can be used realistically in representing the physical descriptors like charge distribution and dipole moments of molecules.

1. Introduction

Electronegativity has been one of the most useful theoretical constructs in chemistry from the early days of the history of science. Though fundamentally a conundrum, the electronegativity concept is widely used by chemists, physicists, biologists and geologists [1,2]. The electron distribution is fundamental in determining the physico-chemical properties of molecules in both ground and excited states. The electronegativity is an important tool in sketching the static distribution and dynamic rearrangement of electronic charge in molecules [3,4]. Although the idea of electronegativity is very old, it was only in 1932 when Pauling [5,6] by his seminal work identified electronegativity with "*the power of an atom in a molecule to attract electrons*" and suggested a scale of its measurement. This definition of electronegativity has been heuristically important and is deeply implanted in minds of chemists even today. The unique idea of Pauling that electronegativity originates from the electron attracting power of bonded atom worked as the guideline in the subconscious mind of all scientists who framed the scales of measurement of electronegativity in the later time. Theoretical chemists have suggested a good number of scales of measurement of electronegativity on the basis of various qualitative conjectures regarding the 'electron attracting power'. There are also reports of small reviews of the concepts and scales of electronegativity [1,2]. A critical analysis of the suggested scales reveals that the best scale of measurement of electronegativity is yet to be designed.

Parr [7], relying upon the definition of electronegativity of Iczkowski and Margrave [8] and within the scope of the new paradigm of quantum mechanics, the density functional theory, derived a quantum mechanical formula of electronegativity. Afterwards, Putz [9-12] made more critical analysis of the concept and measurement of electronegativity from various fundamental standpoints including density functional theory and path integral approach. He has also argued on the possibility of quantum observable of electronegativity [13]. But the fact remains that, since electronegativity is knowable by mind and is not a physical observable; there cannot be any quantum mechanical operator according to the rules of quantum mechanics. Hence, the possibility of the quantum mechanical measurement of electronegativity is ruled out and the definition and measurement of electronegativity must be based upon intuitive reification. It is suggested that the electronegativity is like the unicorn of mythical saga [14] and it exists but can not be seen. It is opined that without the subtle interplay of electronegativity, the whole conceptual structure and the equilibrium in the chemical world will crumble. Thus, when the possibility of quantum mechanical and experimental evaluation of electronegativity is ruled out, there is surge of empirical evaluation through intuitive modeling. Fundamentally the electronegativity is measured as physical mathematical quantity representing as force or potential energy of the screened nuclear charge on the valence electron.

Historically the early scales of measuring electronegativity were proposed by Pauling [5,6], Mulliken [15], Gordy [16] and Allred and Rochow [17]. The scale suggested by Allred and Rochow [17] has been very popular and profusely cited.

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Regarding its fundamental status we must point out that the electronegativity is a free atom ground state property and its dimension is either energy [8,15,16,18-19] or force [17] unit. The majority of the scales of electronegativity rely upon energy unit and so far electronegativity scale of Allred and Rochow is the lone example of electronegativity evaluated in the force unit. In molecular quantum mechanics, there are two distinct approaches, namely those of energy and force, for understanding chemical processes [20].

1.1. The scale of Allred and Rochow

In 1958, Allred and Rochow [17] identified the electronegativity of an atom with the electrostatic field and suggested an ansatz for its evaluation. According to them, one measures the electronegativity by measuring this electrostatic force of attraction between the screened nucleus and an electron from the bonded atom.

$$\chi = \text{Force} = e^2 (Z_{eff})/r^2 \quad (1)$$

Where, χ is the electronegativity, r is the distance between an electron and the nucleus, e is the charge on the electron and Z_{eff} is the charge which is effective at the electron due to the nucleus and its surrounding electrons. In this work [17], the electron was considered to be at the covalent boundary, r, of the atom. It appears that the proposed ansatz was to measure the electronegativity identified as the force of attraction between a nucleus and an electron from a bonded atom. They also proposed a more general linear equation to calculate the electronegativity of the atoms invoking the method of least square fitting and using Pauling's electronegativity values as reference scale. The second ansatz was

$$\chi = 0.359(Z_{eff}/r^2) + 0.744 \quad (2)$$

The entries in equation (2) have the same significance as above. Although the ansatz (1) appears to compute electrostatic force, but χ was measured in all earlier efforts [21-23] by putting charge in atomic units and the distance in angstrom unit. Such a quantity really does not represent force in the real world. Also we have pointed out that the ansatz was least square fitted in reference to Pauling's scale in which the electronegativity is expressed in square root of energy [17]. Thus, it is transparent that, although Allred and Rochow identified electronegativity with the electrostatic force most justifiably, no attempt has ever been made to measure the electronegativity by invoking the ansatz of Allred and Rochow in appropriate dimension of force [24].

Recently, we have critically revisited the electronegativity scale of Allred and Rochow –its fundamental and philosophical structure and operational significance [24]. We have found that the basic philosophy and operational significance of the method is scientifically acceptable. But we are surprised to note that the ansatz of Allred and Rochow has never been invoked to evaluate the electronegativity as a force of the real world. We have computed the electronegativities of the atoms of 103 elements using the ansatz of Allred and Rochow. We [24] have taken special care so that no dimensional mismatch occurs between the conceptual structure and the computational procedure and the evaluated the quantity. The ansatz we have used is the equation (1). Where, χ is electronegativity, e is the electronic charge (esu), r is the most probable radius in cm, Z_{eff} is the effective nuclear charge. Thus electronegativity is computed in proper unit of force. Relying upon the fact the electronegativity is a ground state free atom property, we have posited that the size input in computing electronegativity cannot be the covalent radius and the proper size descriptor should be the absolute or most probable radius of the atom. We have, therefore, computed the electronegativities in force (dynes/electron) unit by invoking the electronegativity ansatz of Allred and Rochow cited above and using the absolute radii [25] and effective nuclear charge of Ghosh *et al.* [26]. It is demonstrated that [24] the newly evaluated scale of electronegativity satisfies the sine qua non of a scale of electronegativity.

Now, although the electronegativity is a conundrum and it is neither a physical observable nor a quantum mechanically determinable quantity, some well known chemico-physical descriptors of molecules are conceived in terms of the electronegativity. The descriptors are charge distribution, dipole moment, atomic polar tensors, bond energy, internuclear distance and force constant etc. While the electronegativity is a conceptual construct, these descriptors occur in the real world. We have linked the electronegativity with the descriptors of real world. In an earlier effort, we have revisited Gordy's scale [27] and discovered some serious dimensional mismatch prevalent in all previous calculations. We have also exploited the set of our electronegativity data computed through revised ansatz of Gordy [27] with proper dimension to evaluate the dipole moments of a number of diatomic molecules [28]. In a similar study, Ghosh's scale of electronegativity [29] has been exploited to evaluate as many as two descriptors of the real world [30,31].

In this report, we have exploited the electronegativity data of our scale [24] to calculate the dipole moments of a series of diatomic molecules. Dipole is an index/descriptor of the asymmetry of charge distribution in molecules. The charge distribution of the hetero nuclear diatomic molecules always generates dipole. The bond character is a common topic in chemistry for the determination of the physical and chemical behaviour of compounds. The simplest way to determine bond character is to use the electronegativity difference between the bonded atoms. Again the dipole moment μ of a diatomic molecule AB has been related to the difference of the two atomic electronegativities ($\chi_B - \chi_A$). The dipole moment in hetero nuclear diatomic molecules has several components [32,33] *i.e.,*

$$\mu = \mu_{atomic} + \mu_{overlap} + \mu_{hybridization} + \mu_{polarization} \quad (3)$$

However, there are two principal components. The first one is bond moment which is developed due to unequal sharing of charge between nuclei goaded by their difference in electronegativities. The second component originates from the asymmetry of charge distribution in lone pair electrons in hybrid orbital. The fact that the lone pair of electrons accommodated in a hybrid orbital acquires asymmetry of charge density distribution and generates atomic dipole was mathematically established by Coulson and Dewar [34,35]. Ghosh and Bhattacharyya [36] have derived quantum mechanical algorithm of dipole moment of molecules. These two components of the dipole moment, we can calculate the bond moment part semi-empirically, but the lone pair contribution to the dipole moment of molecules can only be calculated quantum mechanically and the possibility of empirical evaluation of lone pair contribution of dipole is ruled out.

2. Method of computation

Dipole is a descriptor of the asymmetry of charge distribution. Let us reproduce the quantum mechanical algorithm of Ghosh *et al.* [36] and try to understand the algorithm for computation of molecular dipoles. The permanent quantum mechanical electric dipole moment, μ of the molecule whose electric state is given by Ψ_{el} is

$$\mu = \int \Psi^*_{el}\, d_{op}\, \Psi_{el}\, d\tau \quad (4)$$

Where d_{op} is the quantum mechanical operator of dipole moment. The electric dipole moment operator, d_{op}, for a molecule includes summation over both the electronic and nuclear charges.

$$d_{op} = \sum_{i}(-er_i) + \sum_{\alpha} Z_\alpha e r_\alpha \quad (5)$$

Here, r_α is the vector from the origin to the nucleus of atomic number Z_α and r_i is the vector to the electron i. Since the second term in Eq. (5) is independent of the electronic coordinates, we have

$$\mu = \int \Psi^*_{el} \{\sum_{i}(-er_i)\} \Psi_{el}\, d\tau + \sum_{\alpha} Z_\alpha e r_\alpha \int \Psi^*_{el} \Psi_{el}\, d\tau \quad (6)$$

$$\mu = -e\int(\Psi_{el})^2 \sum_{i} r_i\, d\tau_\alpha + e\sum_{\alpha} Z_\alpha r_\alpha \quad (7)$$

Because of the indistinguishability of the electrons, we can write this expression as

$$\mu = -e\, N\int(\Psi_{el})^2\, r_i\, d\tau + e\sum_{\alpha} Z_\alpha r_\alpha \quad (8)$$

N is the number of electrons in the molecule and r_i is the position vector of electron i. Introducing the electronic probability density, ρ(x,y,z) we write

$$\mu = -e \int\int\int \rho(x, y, z)\, r\, dx\, dy\, dz + e\sum_{\alpha} Z_\alpha r_\alpha \quad (9)$$

Now expanding ρ in terms of the molecular orbitals and then expanding the molecular orbitals, in turn, in terms of the atomic orbitals according to the LCAO-MO SCF scheme and invoking the necessary approximations of Pople's method [37-39], the molecular dipole moments are obtained as a sum of two components.

$$\mu_{total} = \mu_{at} + \mu_{sp} \quad (10)$$

The first term arises from the contribution of net atomic charge densities and second one is the contribution of atomic dipoles resulting from the mixing of s and p orbitals on the same atom center.

2.1. Bond component of dipole moment

It has long been recognized that the dipole moment charge q, of the atoms forming a diatomic molecule can be related to the difference of electronegativities of the two atoms. Mulliken [32] pointed out that, in diatomic molecules, the bond pair moment is the main contributor to the electronic dipole moment of the molecules. There are empirical methods [6,40-41] that compute charge densities on atomic sites of heteronuclear diatomics in terms of electronegativites. In this venture we have calculated the charge densities on atomic sites invoking the empirical methods [6,40-41] and using our electronegativity values [24]. There after we have computed bond moments of some hetero nuclear diatomic molecules through the equation discussed below.

2.2. Computation of bond moment

In physics, the electric dipole moment is a measure of the separation of positive and negative electrical charges in a system of charges i.e. a measure of the charge system's overall polarity. In the simple case of two point charges, one with charge +q and one with charge –q, the electric dipole moment is

$$\mu = q \times d \quad (11)$$

where d is the displacement vector and μ is the electric dipole moment vector generated by bond charge. We have taken a series of diatomics whose bond distances, d are known to a satisfactory accuracy. So the dipoles could be calculated if the q's are known. Let us recast the equation (11) to calculate the dipole in debye unit.

$$\mu = q\, e\, R_e \quad (12)$$

where , μ is the dipole moment of molecules in debye unit, q is the dipole moment charge on atomic site , e represents the electronic charge in esu unit and R_e is the internuclear distance of diatomic molecules in centimeter unit.

We have calculated q's through empirical ansatz suggested by various workers invoking electronegativities of the bonded atoms from our scale under reference. The working formulae to evaluate q are mentioned below:

(1) Pauling's formula: Pauling [6] proposed an ansatz to calculate the ionic character of the bond (i.e. static charge) was as

$$q = 1 - \exp(-(\chi_B - \chi_A)^2/4) \quad (13)$$

where χ_B and χ_A are the atomic electronegativities of atoms B and A, respectively.

(2) Nethercot's formula: Nethercot [40] concluded that q could not be a simple function of electronegativity difference of two atoms and he proposed two formulae [40,42-44] to calculate the dipole moment charges. His proposed ansatzs were

$$q = 1 - \exp(-3(\chi_B - \chi_A)^2/2\chi_{AM}^2) \quad (14)$$

$$q = 1 - \exp(-(\chi_B - \chi_A)^{3/2}/\chi_{GM}^{3/2}) \quad (15)$$

where, χ_{AM} and χ_{GM} are the arithmetic mean(AM) and the geometric mean(GM) of the two atomic electronegativities.

(3) Barbe's formula: Barbe [41] proposed another simple equation to calculate the dipole moment charges of hetero nuclear diatomic molecules. The ansatz which has been proposed by Barbe to calculate the dipole moment charges is as

$$q = (\chi_B - \chi_A) / \chi_B \quad (16)$$

Here, $\chi_B > \chi_A$.

We have used the ansatzs equation (13), (14), (15) and (16) to calculate the dipole moment charges using new set of atomic electronegativities [24] calculated by us very recently. The internuclear distances of diatomic molecules are taken from reference [45-46]. The computed dipole charges on atomic sites of different hetero nuclear diatomic molecules based upon different empirical methods are presented in Table 1. Using these atomic charges, bond moments of as many as eight different series of hetero nuclear diatomic molecules have been calculated and presented in Tables 2–9. For a validity test of our calculated dipole moments, available experimental dipole moments [45] are also presented in Tables 2–9.

Table 1. The computed charge densities on atomic sites of a series of diatomic molecules by different algorithms.

Molecule	q (Barbe)	q (Pauling)	q (Nethercot) (AM)	q (Nethercot) (GM)
LiF	0.984	1	0.996	1
NaF	0.985	1	0.996	1
KF	0.993	1	0.997	1
RbF	0.995	1	0.997	1
CsF	0.996	1	0.997	1
LiCl	0.951	1	0.993	0.999
NaCl	0.953	1	0.993	0.999
KCl	0.980	1	0.996	0.999
RbCl	0.985	1	0.996	1
CsCl	0.988	1	0.997	1
LiBr	0.941	1	0.991	0.999
NaBr	0.944	1	0.992	0.999
KBr	0.976	1	0.996	0.999
RbBr	0.982	1	0.996	0.999
CsBr	0.985	1	0.996	1
LiI	0.920	1	0.987	0.997
NaI	0.923	1	0.988	0.998
KI	0.967	1	0.995	0.999
RbI	0.976	1	0.996	0.999
CsI	0.980	1	0.996	0.999
LiH	0.862	0.999	0.968	0.971
NaH	0.869	0.999	0.971	0.975
KH	0.943	0.999	0.991	0.999
RbH	0.958	0.999	0.994	0.999
CuF	0.955	1	0.993	0.999
AgF	0.967	1	0.995	0.999
AgCl	0.896	1	0.981	0.990
AgBr	0.877	1	0.974	0.981
AgI	0.831	1	0.952	0.944
HF	0.886	1	0.978	0.986
HCl	0.643	1	0.739	0.672
HBr	0.574	1	0.622	0.562
HI	0.417	0.999	0.340	0.332
BrCl	0.161	0.967	0.045	0.071
ICl	0.387	0.999	0.292	0.293
IF	0.805	1	0.934	0.915
IBr	0.269	0.999	0.135	0.162
GeO	0.836	1	0.955	0.949
GeS	0.517	0.999	0.518	0.474
GeSe	0.461	0.999	0.417	0.392
GeTe	0.267	0.874	0.132	0.159
PbO	0.901	1	0.982	0.992
PbS	0.709	1	0.836	0.779
PbSe	0.675	1	0.790	0.725
PbTe	0.558	0.999	0.593	0.537
BaO	0.987	1	0.997	1
NO	0.370	1	0.266	0.272
CO	0.636	1	0.729	0.662

Table 2. The evaluated dipole moments vis-à-vis the experimental dipole moments of a number of alkali halides.

Molecule	Inter nuclear distance, R_e (Å)	Dipole Moment (Barbe) (Debye)	Dipole moment (Pauling) (Debye)	Dipole Moment (Nethercot) (AM) (Debye)	Dipole Moment (Nethercot) (GM) (Debye)	Dipole Moment (Exptl) (Debye)
LiF	1.5638785	7.39	7.51	7.48	7.51	6.32736
NaF	1.9259692	9.11	9.24	9.21	9.24	8.1558
KF	2.1714824	10.35	10.42	10.39	10.42	8.59260
RbF	2.2703609	10.85	10.90	10.87	10.90	8.5465
CsF	2.3453792	11.21	11.26	11.23	11.26	7.8839
LiCl	2.0206913	9.22	9.70	9.63	9.70	7.1289
NaCl	2.3608225	10.80	11.33	11.25	11.33	9.0012
KCl	2.666683	12.54	12.80	12.75	12.80	10.2690
RbCl	2.786769	13.18	13.38	13.33	13.38	10.510
CsCl	2.9063065	13.78	13.95	13.90	13.95	10.387
LiBr	2.021491	9.13	9.70	9.62	9.70	7.2680
NaBr	2.5020676	11.34	12.01	11.91	12.00	9.1183
KBr	2.820809	13.21	13.54	13.48	13.54	10.6278
RbBr	2.9447792	13.88	14.13	14.08	14.13	10.86
CsBr	3.0722875	14.53	14.75	14.69	14.75	10.82
LiI	2.391944	10.56	11.48	11.33	11.45	7.4285
NaI	2.7114844	12.02	13.01	12.86	12.98	9.2357
KI	3.0478794	14.14	14.63	14.55	14.63	10.82
RbI	3.1769183	14.88	15.25	15.18	15.25	11.48
CsI	3.3152313	15.59	15.91	15.85	15.91	11.69

Table 3. The evaluated dipole moments vis-à-vis the experimental dipole moments of some alkali hydrides.

Molecule	Inter nuclear distance, R_e (Å)	Dipole Moment (Barbe) (Debye)	Dipole moment (Pauling) (Debye)	Dipole Moment (Nethercot) (AM) (Debye)	Dipole Moment (Nethercot) (GM) (Debye)	Dipole Moment (Exptl) (Debye)
LiH	1.594	6.60	7.65	7.41	7.43	5.8836
NaH	1.8866	7.86	9.05	8.79	8.83	–
KH	2.24	10.14	10.75	10.66	10.75	–
RbH	2.366808	10.89	11.36	11.29	11.36	–

Table 4. The evaluated dipole moments vis-à-vis the experimental dipole moments of some coinage metal halides.

Molecule	Inter nuclear distance, R_e (Å)	Dipole Moment (Barbe) (Debye)	Dipole moment (Pauling) (Debye)	Dipole Moment (Nethercot) (AM) (Debye)	Dipole Moment (Nethercot) (GM) (Debye)	Dipole Moment (Exptl) (Debye)
CuF	1.7449508	7.999	9.82	8.32	8.37	5.77
AgF	1.983203	9.21	9.52	9.47	9.52	6.22
AgCl	2.280819	9.81	10.95	10.74	10.84	5.70
AgBr	2.393138	10.07	11.49	11.19	11.26	–
AgI	2.544651	10.15	12.21	11.63	11.53	–

Table 5. The evaluated dipole moments vis-à-vis the experimental dipole moments of hydrogen halides.

Molecule	Inter nuclear distance, R_e (Å)	Dipole Moment (Barbe) (Debye)	Dipole moment (Pauling) (Debye)	Dipole Moment (Nethercot) (AM) (Debye)	Dipole Moment (Nethercot) (GM) (Debye)	Dipole Moment (Exptl) (Debye)
HF	0.91682	3.90	8.37	4.30	4.34	1.826526
HCl	1.2745717	3.93	7.80	4.52	4.11	1.1086
HBr	1.4146569	3.90	9.66	4.22	3.81	0.8280
HI	1.609128	3.22	10.25	2.63	2.56	0.4477

Table 6. The evaluated dipole moments vis-à-vis the experimental dipole moments of some interhalogen compounds.

Molecule	Inter nuclear distance, R_e (Å)	Dipole Moment (Barbe) (Debye)	Dipole moment (Pauling) (Debye)	Dipole Moment (Nethercot) (AM) (Debye)	Dipole Moment (Nethercot) (GM) (Debye)	Dipole Moment (Exptl) (Debye)
BrCl	2.136091	1.65	9.92	0.46	0.73	0.57
ICl	2.3209049	4.31	11.14	3.25	3.27	1.24
IF	1.9097813	7.38	9.17	8.56	8.38	–
IBr	2.484801	3.21	11.91	1.61	1.93	–

Table 7. The evaluated dipole moments vis-à-vis the experimental dipole moments of some binary compounds of germanium with chalcogens.

Molecule	Inter nuclear distance, R_e (Å)	Dipole Moment (Barbe) (Debye)	Dipole moment (Pauling) (Debye)	Dipole Moment (Nethercot) (AM) (Debye)	Dipole Moment (Nethercot) (GM) (Debye)	Dipole Moment (Exptl) (Debye)
GeO	1.624667	6.52	7.80	7.45	7.40	–
GeS	2.0120982	4.99	9.66	5.00	4.57	–
GeSe	2.1346561	4.72	10.25	4.27	4.02	1.648
GeTe	2.3401928	2.99	9.82	1.49	1.79	1.06

Table 8. The evaluated dipole moments vis-à-vis the experimental dipole moments of some binary compounds of lead with chalcogens.

Molecule	Inter nuclear distance, R_e (Å)	Dipole Moment (Barbe) (Debye)	Dipole moment (Pauling) (Debye)	Dipole Moment (Nethercot) (AM) (Debye)	Dipole Moment (Nethercot) (GM) (Debye)	Dipole Moment (Exptl) (Debye)
PbO	1.9218359	8.31	9.22	9.06	9.15	4.64
PbS	2.2868898	7.78	10.98	9.18	8.55	3.59
PbSe	2.4022637	7.79	11.53	9.11	8.36	3.28
PbTe	2.595006	6.95 12.45	7.39	6.69		2.73

Table 9. The evaluated dipole moments vis-à-vis the experimental dipole moments of some binary compounds of oxygen.

Molecule	Inter nuclear distance, R_e (Å)	Dipole Moment (Barbe) (Debye)	Dipole moment (Pauling) (Debye)	Dipole Moment (Nethercot) (AM) (Debye)	Dipole Moment (Nethercot) (GM) (Debye)	Dipole Moment (Exptl) (Debye)
BaO	1.9397119	9.19	9.31	9.28	9.31	7.954
NO	1.15074	2.04	5.52	1.47	1.50	0.15872
CO	1.12833632	3.45	5.42	3.95	3.58	0.112

3. Results and Discussion

3.1. Charge distribution on atomic sites

We have set out to apply the force concept of electronegativity to compute some descriptors of the real world and we have chosen to evaluate the dipole moments of a number of suitable chosen hetero nuclear diatomic molecules. We have listed the compounds selected for the present study in Table 1. The dipole charges *i.e.,* the charge densities on atomic sites are computed through four different algorithms laid down above are also presented in Table 1. From chemical experience we can say that the majority of compounds in Table 1 are mostly ionic in nature and formed by the electrostatic force. Surprisingly the atomic charge densities on the atoms are either equal or nearly equal to unity. However, the q's on atoms of the well known covalent compounds like CO and NO is also consistent with the nature of bonding. But Table 1 demonstrates that the dipole charges on atomic sites of CO and NO computed through the ansatz (13) are erroneous. We also note that q's computed through Pauling's ansatz is consistently bad in representing the bonding situation in molecules. Thus the evaluated charge distribution on the atomic sites of a series of diatomic molecules, well known for their ionic character, reveals realistically the physical characteristics of such compounds. The realistic charge distributions revealed through present calculation using the electronegativity scale of Allred and Rochow modified by us [24], unequivocally demonstrates that the revised scale is quite efficacious in revealing and computing charge distribution in molecules. The discrepancy of Pauling's ansatz in computing the dipole charges noted by Nethercot [40] is once again evident here.

3.2. Dipole moment

The dipole moments of the predominantly ionic compounds are presented in Tables 2–4 and for covalent compounds are presented in Tables 5-9. From the Table 2 it is distinct that calculated dipole moments of alkali halides show a nice correlation with the experimental dipole moments. From Table 1 and our chemical experience predict that the compounds in Table 2 are grossly ionic and hence the bond moments are expected to be high. We have presented the computed dipole moments of hydrides of Li, Na, K and Rb along with the available experimental value in Table 3. From Table 1 and from our chemical experience we can infer that the hydrides of such metals as are studied here are mostly ionic and the computed dipoles should be accordingly high. We have

presented the computed dipoles of another series of ionic compounds in Table 4. The computed dipoles of five coinage metal halides are presented in Table 4. Table 1 reveals that the dipole charges computed through Pauling's formula is systematically deviated from the chemical physical characteristics of such compounds. But the dipole charges evaluated through other three methods are satisfactory. Table 4 demonstrates that the magnitude of dipole moments are high reflecting the ionic character of bonds and the variation of dipoles in the series is also consistent with the physical nature of the bonds of such molecules. A closer look into the Tables 2–4 reveals that the theoretically evaluated and experimental bond moments of number of molecules are systematically high in magnitude and have a good correlation between the two sets of dipole data.

The dipole moment data of predominantly covalent compounds are presented in Tables 5–9. We can observe from the Table 5 that, in case of hydrogen halides, the calculated dipole moments using the ansatz of Pauling shows larger deviations from experimental values consistent to our above observation. But dipoles computed through other three formulae of Nethercot and Barbe, the equations (14), (15), (16) respectively, have good correlation with their experimental counter parts.

The dipole moments of some diatomic interhalogen compounds are presented in Table 6. A close look at the Table 6 reveals that the computed dipoles of the inter halogen compounds have good agreement with the experimental results.

The computed dipoles of the diatomic compounds of Ge and Pb with the Group-16 elements are presented in the Table 7 and 8 respectively along with their experimental counter parts. From Table 1 it is distinct that the degree of covalency of the chalcogenides of Ge and Pb, consistent with our common experience gathered from the chemico-physical behaviour of such compounds revealed through the chemical literature, is increasing with the increasing atomic number of chalcogens. Again, Table 1 shows that the dipoles charge of chalcogenides of Ge and Pb are very poorly and erroneously represented by the Pauling's method of evaluating dipole charges. Table 7 demonstrates that the nature of the dipoles of chalcogenides of Ge computed by invoking the ansatz of Barbe and Nethercot (columns III, V and VI) are consistent with the well known increasing covalency of such compounds in the series. The corresponding result in Pauling's method is inconsistent with the known physical situation. The known variation of the physico-chemical nature of the chalcogenides of Pb is that the degree of covalency in such compounds increases downward in the series. Table 8 demonstrates that, consistent with their chemico-physical nature, the dipoles of the chalcogenides of Pb decrease systematically in the series in the theoretical as well as experimental evaluation. The dipoles computed through Pauling;s formula is, however, consistently inconsistent. The experimental dipoles of chalcogenides of Pb are significantly small compared to the theoretical evaluation. Table 9 exhibits the dipole moments a series of compounds having strongly ionic character to strongly covalent character. In Table 9 we have presented the oxides of Ba, C and N along their computed and experimental dipole moments. From Table 1 we see that dipole charges are realistically estimated in all method except that of Pauling's formula. It is transparent from the Table 9 that when the ionic oxide of barium has higher value of dipole moment, the covalent molecules CO and NO possess lower dipole values. The calculated q values for these covalent oxides also justify our observation. The experimental dipole moments of BaO, CO and NO (Table 9) follow pattern of the variation of the dipole charges reported in Table 1. A closer look into the Tables 5–9 reveals that there is a systematic discrepancy between theoretically evaluated and experimental bond moments of covalent compounds. This behaviour is not at all undesirable in view of the fact the dipole of ionic compounds can be computed through equation (12). The ions are spherically symmetrical and dipoles due asymmetry of charge distribution in hybrid orbitals will be absent. But with increasing covalency, the equation (12) can not evaluate dipoles rather the appropriate algorithm should be the equation (10).

4. Conclusions

Although electronegativity is neither a physical observable nor a quantum mechanically determinable quantity, it is a very useful theoretical constructs in chemistry and physics and can be linked to a number of descriptors of the real world. In this work, we report the computation of dipole moments of diverse nature molecules ranging between strongly ionic to strongly covalent in terms of the electronegativity computed within the paradigm of force concept. We have used the available ansatz for computing the charge densities on atomic sites and dipole moments. The electronegativities used are computed by us using the basic force concept approach of Allred and Rochow but allaying seemingly dimensional mismatch in all previous calculations. The dipole charges are quite consistent with the known chemico-physical nature of the compounds brought under investigation. The computed dipole moments are realistic descriptors of the charge distribution in the molecules under study. The nature of variation of bonds from strongly covalent to strongly ionic is well reflected in the computed dipole charges and also in the evaluated dipole moments. The correlation between the theoretical dipole moments and the available experimental dipole moments are satisfactory. Thus, our scale of electronegativity is quite successful in computing charge distribution in molecules realistically.

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